Rapid Communications

# Spin Hartree-Fock approach to studying quantum Heisenberg antiferromagnets in low dimensions

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We construct a new mean-field theory for a quantum (spin-1/2) Heisenberg antiferromagnet in one (1D) and two (2D) dimensions using a Hartree-Fock decoupling of the four-point correlation functions. We show that the solution to the self-consistency equations based on two-point correlation functions does not produce any unphysical finite-temperature phase transition, in accord with the Mermin-Wagner theorem, unlike the common approach based on the mean-field equation for the order parameter. The next-neighbor spin-spin correlation functions, calculated within this approach, reproduce closely the strong renormalization by quantum fluctuations obtained via a Bethe ansatz in 1D and a small renormalization of the classical antiferromagnetic state in 2D. The heat capacity approximates with reasonable accuracy the full Bethe ansatz result at all temperatures in 1D. In 2D, we obtain a reduction of the peak height in the heat capacity at a finite temperature that is accessible by high-order $1/T$ expansions.

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Interest in low-dimensional quantum antiferromagnets has been revived in the last decades by the discovery of high-$T_c$ superconductors, where the physics of the quantum spin fluctuations on a square lattice was suggested to be the main mechanism behind superconductivity [1]. More recently, the magnetic properties of insulators such as $Cs_2CuCl_4$ [2,3], $CsNiCl_3$ [4], and $Cs_2CuBr_4$ [5], where at low temperatures a moderate degree of anisotropy (about 0.3–0.4) makes their dimensionality intermediate between one and two, have caused a new resurgence of activity in this problem. In both cases the dimensionality is smaller than three, where the classical long-range order in the ground state was rigorously proven [6,7], but is bigger than strictly one, making the exact Bethe ansatz solution [8] inapplicable. Thus, a more accurate description of the effect of quantum fluctuations is required, which become strong in reduced dimensions, and for the quantum spin $S = 1/2$.

A popular method to deal with low-dimensional quantum spin systems is Takahashi's modified spin-wave theory that was quite successful, especially for ferromagnets, where it, for instance, at low temperature, reproduces correctly the subleading terms of the free energy [9] obtained using the thermodynamic Bethe ansatz approach [10,11]. Generally, this and other predictions of Takahashi's theory are almost equivalent to the Schwinger-boson mean-field theory formulated by Arovas and Auerbach [12] and to the one-loop renormalization group calculations [13]. However, at high temperatures, the spin-wave result for the free energy is divergent [9], disagreeing entirely with the high-temperature expansion in its limit of validity. In the antiferromagnetic case, predictions of the modified spin-wave theory are not as good for $S = 1/2$. In one dimension (1D), they lead to a gapful ground state and an exponential two-point correlation function at zero temperature that deviates strongly from the known Bethe ansatz gapless ground state [8] and algebraic correlations [14–17] at zero temperature. Also, in both 1D and 2D, there is a spurious finite-temperature phase transition within the spin-wave approach, which is explicitly forbidden in these dimensions by the Mermin-Wagner theorem [18]. The latter problem stems from the need of introducing two sublattices in the construction of the spin-wave theory in the antiferromagnetic case [12,19], which is based on the simplest mean-field approximation using the sublattice magnetization (a one-point correlation function) as the order parameter and causes an order-disorder phase transition in all dimensions that is not washed out by spin waves.

In this Rapid Communication, we construct an alternative mean-field approach for the spin-1/2 antiferromagnet in 1D and 2D based on the decoupling of the four-point correlation functions. The corresponding self-consistency equations are derived using the Hartree-Fock decoupling for the Heisenberg interactions and assuming the exclusive statistics of free magnons. It recovers almost all effects of the strong renormalization of the classical spin picture in 1D at low temperatures established by the Bethe ansatz, including the heat capacity and the static correlation functions, with the most notable exception of the logarithmic contribution to the magnetic susceptibility that is driven by the low-energy physics of the Luttinger liquid and requires taking into account even higher-order correlation functions. At high temperatures, our method recreates the $1/T$ expansion and produces no phase transition at intermediate temperatures. In 2D, the same approach recovers only a small renormalization of the classical antiferromagnetic state [20] in the next-neighbor spin-spin correlation function and the high-temperature expansion, producing again no finite-temperature phase transition. The height of a smooth peak (instead of a transition) at an intermediate temperature, for instance, in the heat capacity, is reduced in 2D with respect to its value in 1D that is still accessible via a high-order $1/T$ expansion in 2D [21,22] and is already captured qualitatively on the level of the two-point correlation functions. The biggest quantitative discrepancy of ignoring three- and higher-point correlation functions occurs at intermediate temperatures and is of the

 

order of 20% in 1D, where the thermodynamic quantities can be calculated at arbitrary temperatures [23–26] using the thermodynamic Bethe ansatz [10,11].

We study the Heisenberg model for spin-1/2 in the presence of an external magnetic field $B$, in one ($D = 1$) and two ($D = 2$) dimensions,

$$H = B\sum_{\mathbf{r}} S^z_{\mathbf{r}} + \frac{J}{2}\sum_{\mathbf{r},\delta} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\delta}, \tag{1}$$

where $J$ is the exchange energy, $S^z_{\mathbf{r}}, S^{\pm}_{\mathbf{r}} = S^x_{\mathbf{r}} \pm i S^y_{\mathbf{r}}$ are the spin-1/2 operators at site $\mathbf{r}$, the sum over $\mathbf{r}$ runs over an equidistant (square) lattice consisting of $N = L^D$ spins in 1D (2D), and the sum over $\delta$ runs over two or four nearest neighbors in the corresponding dimension. Below, we impose periodic boundary conditions, $\mathbf{S}_{\mathbf{r}+\mathbf{x}(\mathbf{y})L} = \mathbf{S}_{\mathbf{r}}$, restrict ourselves to the antiferromagnetic exchange energy $J > 0$, and use the units where $g\mu_B = 1$.

Before proceeding with solving the model in Eq. (1), we reduce the number of the spin components in it by utilizing the following spin-1/2 identity, $S^z_{\mathbf{r}} = S^+_{\mathbf{r}} S^-_{\mathbf{r}} - 1/2$. This turns the Zeeman term in the Hamiltonian into a quadratic form and the $z$ component of the scalar product into a quartic form, expressing Eq. (1) in terms of only $S^{\pm}_{\mathbf{r}}$ operators.

In the Fourier domain, $S^{\pm}_{\mathbf{r}} = N^{-1/2}\sum_{\mathbf{k}} S^{\pm}_{\mathbf{k}} e^{\pm i\mathbf{k}\cdot\mathbf{r}}$, the resulting Hamiltonian becomes a sum of a quadratic and a quartic form in the single spin operators,

$$H = \sum_{\mathbf{k}} (B - DJ + \varepsilon_{\mathbf{k}}) S^+_{\mathbf{k}} S^-_{\mathbf{k}} + \frac{1}{N}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_3,\mathbf{k}_2+\mathbf{k}_4} \varepsilon_{\mathbf{k}_3-\mathbf{k}_4} S^+_{\mathbf{k}_1} S^-_{\mathbf{k}_2} S^+_{\mathbf{k}_3} S^-_{\mathbf{k}_4}, \tag{2}$$

where the dispersion is $\varepsilon_{\mathbf{k}} = J\sum_{\alpha} \cos k_{\alpha}$, the sum $\sum_{\alpha}$ contains only one term $\alpha = x$ in 1D and it runs over two spatial dimensions, $\sum_{\alpha=x,y}$, in 2D, and the sum over momentum $\sum_{\mathbf{k}}$ also runs over one ($k$) or two ($k_x$,$k_y$) components of the wave vector in the corresponding dimension.

In order to analyze the model in Eq. (2) we assume that its eigenstates factorize in the momentum domain, i.e., they can be approximated by product states of single magnon excitations in the thermodynamic limit [27]. At a finite temperature this approach corresponds to writing down the following product density matrix, $\rho = \prod_{\mathbf{k}} [m_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}| + (1 - m_{\mathbf{k}})]$, where $|\mathbf{k}\rangle$ is a single magnon state at a given $\mathbf{k}$, exclusive statistics for the states with different $\mathbf{k}$ is implied [30], $m_{\mathbf{k}}$ are scalar parameters, and the normalization is chosen as $\mathrm{Tr}\,\rho = 1$. We believe that this density matrix gives a close enough approximation to the many-magnon states. The expectation value of the Hamiltonian in Eq. (2) with respect to this $\rho$ gives the energy of the system $E = \langle H\rangle$ as a function of parameters $m_{\mathbf{k}}$,

$$E = \sum_{\mathbf{k}} (B - DJ + \varepsilon_{\mathbf{k}}) m_{\mathbf{k}} - \frac{1}{N}\sum_{\mathbf{k}_1\mathbf{k}_2} \varepsilon_{\mathbf{k}_1-\mathbf{k}_2} m_{\mathbf{k}_1} m_{\mathbf{k}_2}, \tag{3}$$

where the contribution of the terms with $\mathbf{k}_1 = \mathbf{k}_2$ in the second line vanishes in the $N \to \infty$ limit and the average of an operator is $\langle\cdots\rangle = \mathrm{Tr}(\rho\cdots)$. The second term in Eq. (3) is equivalent to the Hartree-Fock approximation to the quartic interaction term in Eq. (2), $\langle S^+_{\mathbf{k}_1} S^-_{\mathbf{k}_2} S^+_{\mathbf{k}_3} S^-_{\mathbf{k}_4}\rangle \approx m_{\mathbf{k}_1} m_{\mathbf{k}_3} \delta_{\mathbf{k}_1,\mathbf{k}_2}\delta_{\mathbf{k}_3,\mathbf{k}_4} + m_{\mathbf{k}_1}(1 - m_{\mathbf{k}_2})\delta_{\mathbf{k}_1,\mathbf{k}_4}\delta_{\mathbf{k}_2,\mathbf{k}_3}$, where the first term is the direct and the second is the exchange part. The average of the operator $S^+_{\mathbf{k}} S^-_{\mathbf{k}}$ in the first term in Eq. (2) gives the scalar parameter $\langle S^+_{\mathbf{k}} S^-_{\mathbf{k}}\rangle = m_{\mathbf{k}}$ that can be interpreted as a two-point correlation function. The inverse Fourier transform gives the correlation function $\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} m_{\mathbf{k}}/N = \langle S^+_{\mathbf{r}} S^-_{\mathbf{0}}\rangle$, where $\mathbf{0}$ is a reference point on the lattice in 1D and 2D and the translational invariance of the model in Eq. (1) was used.

The values of the mean-field parameters $m_{\mathbf{k}}$ at a finite temperature $T$ can be found in the usual way by minimizing the free energy, $F = E - TS$, with respect to them. The energy $E$ is given by Eq. (3) and the von Neumann entropy, $S = -k_B\,\mathrm{Tr}(\rho\ln\rho)$, is given by $-k_B\sum_{\mathbf{k}}[m_{\mathbf{k}}\ln m_{\mathbf{k}} + (1 - m_{\mathbf{k}})\ln(1 - m_{\mathbf{k}})]$, where $k_B$ is the Boltzmann constant. Solving $\partial F/\partial m_{\mathbf{k}} = 0$, we obtain the mean-field self-consistency equations as

$$m_{\mathbf{k}} = \frac{1}{e^{\beta(B - DJ + \varepsilon_{\mathbf{k}} - \frac{2}{N}\sum_{\mathbf{k}'}\varepsilon_{\mathbf{k}-\mathbf{k}'} m_{\mathbf{k}'})} + 1}, \tag{4}$$

where $\beta = 1/(k_B T)$ is the inverse temperature. The above is a large set of $N$ nonlinear equations for the mean-field parameters $m_{\mathbf{k}}$. However, the $m_{\mathbf{k}}$ enter in the exponential function only under a sum. Thus, the number of independent nonlinear equations can be reduced greatly. We introduce $1 + D$ extensive variables as $s = \sum_{\mathbf{k}} m_{\mathbf{k}}/N - 1/2$ and $u_{\alpha} = -\sum_{\mathbf{k}} m_{\mathbf{k}} \cos k_{\alpha}/N + 1/2$, where $u_{\alpha} = u$ is a scalar in 1D and $u_{\alpha} = (u_x, u_y)$ is a vector in 2D. Substituting these definitions into Eq. (4), we express its right-hand side in terms of only $s$ and $u_{\alpha}$, and then substituting the resulting expressions for $m_{\mathbf{k}}$ back into the definitions for $s$ and $u_{\alpha}$, we rewrite Eq. (4) as a set of only $1 + D$ independent equations,

$$s = \int \frac{d^D k}{(2\pi)^D} \frac{1}{e^{\beta(B + 2DJs + 2J\sum_{\alpha} u_{\alpha}\cos k_{\alpha})} + 1} - \frac{1}{2}, \tag{5}$$

$$u_{\alpha} = \frac{1}{2} - \int \frac{d^D k}{(2\pi)^D} \frac{\cos k_{\alpha}}{e^{\beta(B + 2DJs + 2J\sum_{\alpha} u_{\alpha}\cos k_{\alpha})} + 1}, \tag{6}$$

where the sum over $\mathbf{k}$ was turned into an integral in the thermodynamic limit as $\sum_{\mathbf{k}}/N \to \int d^D k/(2\pi)^D$ [31]. Here, the parameter $s$ gives the average magnetization per spin as $\sum_{\mathbf{r}}\langle S^z_{\mathbf{r}}\rangle/N = s$ and the parameter $u_{\alpha}$ is related to the kinetic energy of magnons.

There is only one nontrivial solution of Eqs. (5) and (6). Let us analyze it at $B = 0$. At zero temperature the integrands are proportional to the Heaviside step function $\lim_{\beta\to\infty}[\exp(\beta x) + 1]^{-1} = \Theta(-x)$, then the integrals can be calculated explicitly, and we obtain $s = 0$ (unpolarized ground state) and $u_x = u_y = 1/2 + D/\pi^D$. On the other hand, at high temperatures, the exponential expands into a Taylor series in $\beta \ll 1$ up to the leading order as $[\exp(\beta x) + 1]^{-1} = 1/2 + O(\beta)$ and we get $s = 0$ and $u_x = u_y = 1/2$. At intermediate temperatures, the equations can be solved numerically.

The thermodynamic quantities can be expressed through solutions of Eqs. (5) and (6) at different temperatures and magnetic fields. The energy in Eq. (3) can be written as a function of $s$ and $u_{\alpha}$ using their definitions in terms of $m_{\mathbf{k}}$, $E = N(Bs + DJs^2 - J\sum u_{\alpha}^2)$, from which, using the basic definition of the heat capacity, we obtain

$$\frac{C}{N} = \frac{1}{N}\frac{\partial E}{\partial T} = (B + 2DJs)\frac{\partial s}{\partial T} - 2J\sum_{\alpha} u_{\alpha}\frac{\partial u_{\alpha}}{\partial T}. \tag{7}$$

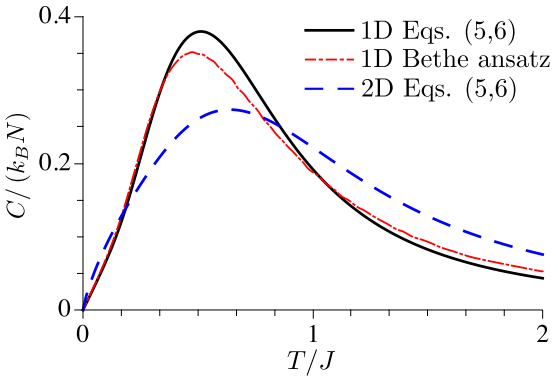


FIG. 1. Specific heat as a function of temperature at $B = 0$ in 1D and 2D. The solid black and the blue dashed lines are obtained by solving the self-consistency Eqs. (5) and (6) and the heat capacity by means of Eq. (7). The red dashed-dotted line is the exact result of the thermodynamic Bethe ansatz calculation in 1D from Ref. [26].

The temperature dependence of $C$ in 1D and in 2D (at $B = 0$) is plotted in Fig. 1. In 1D we can compare our result with the full quantum mechanical result obtained via the thermodynamic Bethe ansatz machinery [10,11] in Refs. [23,24,26]. Up to the intermediate temperatures, Eqs. (5) and (6) agree quite well with it, including the linear dependence of $C$ at low temperatures. Equations (5) and (6) also reproduce correctly the coefficient of the leading term of the $1/T$ expansion at high temperatures. However, in the intermediate-temperature region, from $T \geqslant J/2$, the difference (see the black solid and the red dashed-dotted lines in Fig. 1) is still appreciable, up to 20%. In 2D, Eqs. (5) and (6) produce no phase transition at any finite temperature, in agreement with the Mermin-Wagner theorem [35], and that has already been seen in a quantum Monte Carlo study [36]. Also, the high-order $1/T$ expansion [21] covers a significant temperature range down to the peak, whose amplitude is reduced with respect to the 1D case. The result of solving Eqs. (5) and (6) (the blue dashed line in Fig. 1) gives about the same discrepancy of up to 20% with Ref. [21] in the intermediate-temperature region.

This discrepancy can be understood in terms of improving the approximate description of the Heisenberg model by taking into account higher-order correlation functions. The usual way of introducing the mean-field approximation to the model in Eq. (1) is by retaining only the one-point correlation functions $\langle S^z_{\mathbf{r}}\rangle = \pm m$, where $m$ is the order (a single mean-field) parameter and $\pm$ describes the even/odd sublattice of the antiferromagnet. Neglecting the quadratic terms in fluctuations around $\langle S^z_{\mathbf{r}}\rangle$ (and assuming that $\langle S^{\pm}_{\mathbf{r}}\rangle = 0$) in Eq. (1), the usual self-consistency equations are the same for each sublattice for $B = 0$,

$$2m = \tanh(\beta D J m). \tag{8}$$

This equation does predict the antiferromagnetic order at $T = 0$, but it also introduces an erroneous phase transition at a finite $T$ in low dimensions, which is explicitly forbidden by the Mermin-Wagner theorem [18]. In the present work, we take into account the two-point correlation function solving the self-consistency equations in Eq. (4) for $N$ mean-field parameters $m_{\mathbf{k}}$. This approach contains more information about the quantum fluctuations, which play a stronger role in low dimensions, improving the approximation qualitatively, i.e., not introducing a finite-$T$ phase transition, and quantitatively, as illustrated in 1D by comparison with the Bethe ansatz in Fig. 1. An approach that accounts for higher than two-point correlation functions would improve the accuracy even further.

Another thermodynamic quantity that is of interest in magnets is the magnetic susceptibility $\chi = \partial(\sum_{\mathbf{r}}\langle S^z_{\mathbf{r}}\rangle)/\partial B$. Using as before the identity $S^z_{\mathbf{r}} = S^+_{\mathbf{r}} S^-_{\mathbf{r}} - 1/2$ and the definition of $s$ in terms of $m_{\mathbf{k}}$, we obtain $\chi = N\partial s/\partial B$. The temperature dependence of this result at $B = 0$ shows a better [in comparison with the more crude approximation in Eq. (8)] agreement with the full Bethe ansatz calculation [25,26], both quantitatively and qualitatively. However, there are larger deviations at small temperatures, unlike for the heat capacity, due to the logarithmic corrections [25]. They are essentially an effect of Luttinger physics manifesting hydrodynamic modes which are not captured on the level of the two-point correlation functions in Eq. (4).

The static correlation functions can also be calculated in terms of the solutions of Eqs. (5) and (6). Expressing the operator $\mathbf{S_0}\cdot\mathbf{S_r}$ in the Fourier domain and evaluating its finite-temperature average using $\rho$ in the same way as in the calculation of the energy of the system in Eq. (3), we obtain

$$\langle \mathbf{S_0}\cdot\mathbf{S_r}\rangle = s^2 + I(\mathbf{r})[1 - I(\mathbf{r})], \tag{9}$$

where

$$I(\mathbf{r}) = \int \frac{d^D k}{(2\pi)^D} \frac{\cos(\mathbf{k}\cdot\mathbf{r})}{e^{\beta(B+2DJs+2J\sum_\alpha u_\alpha \cos k_\alpha)} + 1}. \tag{10}$$

Here, $m_{\mathbf{k}}$ were expressed through $s$ and $u_\alpha$ using their definitions above. For the next-neighbor correlation function the integral in Eq. (10) simplifies even further using Eq. (6), $I(1) = 1/2 - u$ and $I(\mathbf{x}) = 1/2 - u_x$ in the corresponding dimension. At zero temperature we can substitute the already obtained solutions of Eqs. (5) and (6), $s = 0$ and $u_x = u_y = 1/2 + D/\pi^D$, directly. In 1D, where quantum fluctuations play a significant role, we obtain $\langle \mathbf{S}_0\cdot\mathbf{S}_1\rangle = -0.4196\ldots$ that is close to the full Bethe ansatz result $\langle \mathbf{S}_0\cdot\mathbf{S}_1\rangle = -0.4431\ldots$ [37]. In two dimensions we obtain $\langle \mathbf{S_0}\cdot\mathbf{S_x}\rangle = -0.2437\ldots$ that is close to the value of $-1/4$ for the classical antiferromagnet, with only a small reduction due to quantum fluctuations [20].

Beyond the next neighbor the integral in Eq. (10) needs to be calculated explicitly. At $T = 0$ it gives $I(r) = \sin(\pi r/2)/(\pi r)$ in 1D, resulting in the correlation function $\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle = \sin(\pi r/2)/(\pi r)$ at $r \gg 1$. This $1/r$ behavior coincides with the prediction of a Gaussian conformal field theory [14,38] that was confirmed by a direct Bethe ansatz calculation of the corresponding form factors [15–17]. At a finite $T > 0$, a numerical solution of Eqs. (5) and (6) and a numerical evaluation of the integral in Eq. (10) reproduce the expected exponential behavior $|\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle| \propto \exp(-r/\xi)$ at large distances (see the fit in the inset in Fig. 2), where the correlation length in 1D also obtained by fitting is an algebraic function of temperature,

$$\xi = \frac{J}{2T} \tag{11}$$

(see the main part in Fig. 2). This coincides with the $1/T$ behavior obtained using the thermodynamic Bethe ansatz approach [24]. The exponential behavior crosses over into

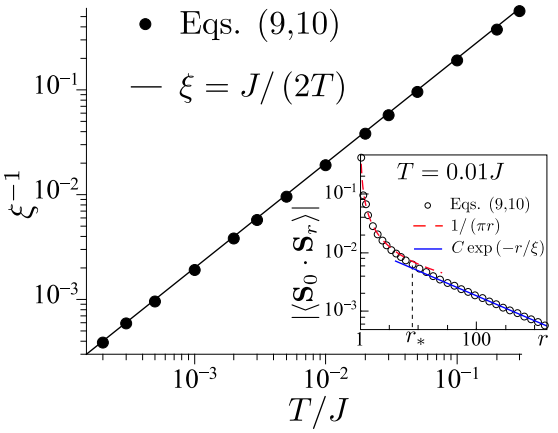


FIG. 2. The static correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$ in 1D evaluated by solving the self-consistency equation in Eqs. (5) and (6) and using Eqs. (9) and (10). The main plot is the temperature dependence of the correlation length $\xi$ in the exponential regime $r > r_*$ obtained numerically (solid circles) and the $1/T$ result of the Bethe ansatz (black line). The inset is the correlation function for an intermediate temperature $T = 0.01J$ obtained numerically (open circles); the zero-temperature result $1/r$ is valid in the short-range region $r < r_*$ (dashed red line) and an exponential, $\exp(-r/\xi)$, is valid in the long-range region $r > r_*$ (solid blue line).

the power law at a finite range $r_*$ (see the inset in Fig. 2), whose value changes smoothly from $r_* = \infty$ at $T = 0$ to $r_* \approx 0$ at $T \simeq J$. In 2D the integral in Eq. (10) gives $I(r\mathbf{x}) = -2\sin(\pi r/2)/(\pi r)^2$ at zero temperature and the $\langle \mathbf{S_0} \cdot \mathbf{S}_{\mathbf{x}r} \rangle = -2\sin(\pi r/2)/(\pi r)^2$ correlation function at $r \gg 1$. At finite temperature the correlation length in the two-dimensional antiferromagnet is known to have an exponential dependence on temperature, $\xi \propto \exp(\text{const}/T)$ [39,40]. Numerically, we find that the result of Eqs. (5), (6), and (10) is consistent with Ref. [39] at a small temperature range below $T \simeq J$, which is still accessible due to not so large values of $r_*$ at relatively not so low temperatures.

In conclusion, we have constructed a mean-field approach based on two-point correlation functions for spin-1/2 antiferromagnets in 1D and 2D, for which the effect of quantum fluctuations is the strongest. Solutions of the corresponding self-consistency equations recover the strong renormalization of the classical spin picture in 1D, established by the Bethe ansatz, and only a small correction to the classical antiferromagnet in 2D. This approach produces no finite-temperature phase transitions, in accord with the Mermin-Wagner theorem, and the $1/T$ expansion at high temperatures in $D = 1$ and $D = 2$. The biggest quantitative discrepancy of ignoring three- and higher-point correlation functions occurs at intermediate temperatures and is up to ∼20% that can be assessed in 1D, where the thermodynamic quantities can be calculated at arbitrary temperatures using the thermodynamic Bethe ansatz. The controversy about the effect of dimensionality in the anisotropic 2D quantum antiferromagnets, e.g., $Cs_2CuCl_4$ (the ratio of the exchange constants is $J_\perp/J_\parallel \simeq 0.33$) for which neutron scattering shows both signatures of one-dimensional physics [41] and a dispersion in the perpendicular direction [42], can be explained here as a dimensional crossover, where strong effects of quantum fluctuations in 1D disappear smoothly as the coupling between the chains is increased.

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